



Full wwPDB EM Validation Report ⓘ

Dec 19, 2023 – 12:59 pm GMT

PDB ID : 8PPT
EMDB ID : EMD-17815
Title : Pyrococcus abyssi DNA polymerase D (PolD) in its editing mode bound to a primer/template substrate containing a mismatch
Authors : Betancurt-Anzola, L.; Martinez-Carranza, M.; Zatopek, K.M.; Gardner, A.F.; Sauguet, L.
Deposited on : 2023-07-10
Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

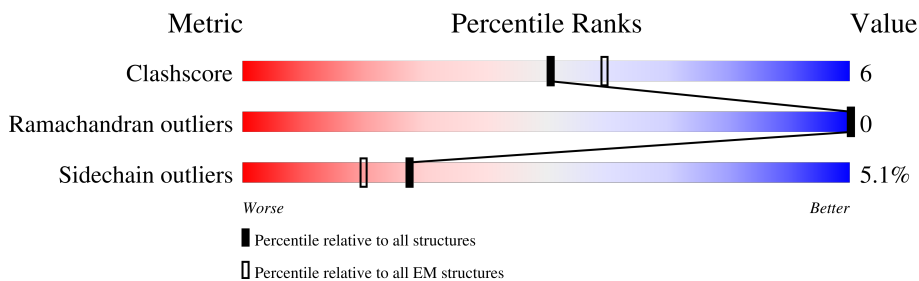
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	662	
2	C	261	
2	D	261	
2	E	261	
3	P	18	
4	T	25	
5	B	1270	

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 19620 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase II small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	447	3565	2319	590	649	7	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP Q9V2F3
A	-41	GLY	-	expression tag	UNP Q9V2F3
A	-40	LYS	-	expression tag	UNP Q9V2F3
A	-39	HIS	-	expression tag	UNP Q9V2F3
A	-38	HIS	-	expression tag	UNP Q9V2F3
A	-37	HIS	-	expression tag	UNP Q9V2F3
A	-36	HIS	-	expression tag	UNP Q9V2F3
A	-35	SER	-	expression tag	UNP Q9V2F3
A	-34	GLY	-	expression tag	UNP Q9V2F3
A	-33	HIS	-	expression tag	UNP Q9V2F3
A	-32	HIS	-	expression tag	UNP Q9V2F3
A	-31	HIS	-	expression tag	UNP Q9V2F3
A	-30	THR	-	expression tag	UNP Q9V2F3
A	-29	GLY	-	expression tag	UNP Q9V2F3
A	-28	HIS	-	expression tag	UNP Q9V2F3
A	-27	HIS	-	expression tag	UNP Q9V2F3
A	-26	HIS	-	expression tag	UNP Q9V2F3
A	-25	HIS	-	expression tag	UNP Q9V2F3
A	-24	SER	-	expression tag	UNP Q9V2F3
A	-23	GLY	-	expression tag	UNP Q9V2F3
A	-22	SER	-	expression tag	UNP Q9V2F3
A	-21	HIS	-	expression tag	UNP Q9V2F3
A	-20	HIS	-	expression tag	UNP Q9V2F3
A	-19	HIS	-	expression tag	UNP Q9V2F3
A	-18	THR	-	expression tag	UNP Q9V2F3
A	-17	SER	-	expression tag	UNP Q9V2F3
A	-16	SER	-	expression tag	UNP Q9V2F3
A	-15	SER	-	expression tag	UNP Q9V2F3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	expression tag	UNP Q9V2F3
A	-13	SER	-	expression tag	UNP Q9V2F3
A	-12	THR	-	expression tag	UNP Q9V2F3
A	-11	GLY	-	expression tag	UNP Q9V2F3
A	-10	GLU	-	expression tag	UNP Q9V2F3
A	-9	ASN	-	expression tag	UNP Q9V2F3
A	-8	LEU	-	expression tag	UNP Q9V2F3
A	-7	TYR	-	expression tag	UNP Q9V2F3
A	-6	PHE	-	expression tag	UNP Q9V2F3
A	-5	GLN	-	expression tag	UNP Q9V2F3
A	-4	GLY	-	expression tag	UNP Q9V2F3
A	-3	THR	-	expression tag	UNP Q9V2F3
A	-2	GLY	-	expression tag	UNP Q9V2F3
A	-1	ASP	-	expression tag	UNP Q9V2F3
A	0	GLY	-	expression tag	UNP Q9V2F3
A	1	SER	-	expression tag	UNP Q9V2F3
A	451	ALA	HIS	engineered mutation	UNP Q9V2F3

- Molecule 2 is a protein called DNA polymerase sliding clamp.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	246	Total	C	N	O	S	0	0
			1939	1238	308	384	9		
2	D	246	Total	C	N	O	S	0	0
			1939	1238	308	384	9		
2	E	246	Total	C	N	O	S	0	0
			1939	1238	308	384	9		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	MET	-	initiating methionine	UNP Q9UYX8
C	-10	ARG	-	expression tag	UNP Q9UYX8
C	-9	GLY	-	expression tag	UNP Q9UYX8
C	-8	SER	-	expression tag	UNP Q9UYX8
C	-7	HIS	-	expression tag	UNP Q9UYX8
C	-6	HIS	-	expression tag	UNP Q9UYX8
C	-5	HIS	-	expression tag	UNP Q9UYX8
C	-4	HIS	-	expression tag	UNP Q9UYX8
C	-3	HIS	-	expression tag	UNP Q9UYX8
C	-2	HIS	-	expression tag	UNP Q9UYX8
C	-1	GLY	-	expression tag	UNP Q9UYX8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q9UYX8
D	-11	MET	-	initiating methionine	UNP Q9UYX8
D	-10	ARG	-	expression tag	UNP Q9UYX8
D	-9	GLY	-	expression tag	UNP Q9UYX8
D	-8	SER	-	expression tag	UNP Q9UYX8
D	-7	HIS	-	expression tag	UNP Q9UYX8
D	-6	HIS	-	expression tag	UNP Q9UYX8
D	-5	HIS	-	expression tag	UNP Q9UYX8
D	-4	HIS	-	expression tag	UNP Q9UYX8
D	-3	HIS	-	expression tag	UNP Q9UYX8
D	-2	HIS	-	expression tag	UNP Q9UYX8
D	-1	GLY	-	expression tag	UNP Q9UYX8
D	0	SER	-	expression tag	UNP Q9UYX8
E	-11	MET	-	initiating methionine	UNP Q9UYX8
E	-10	ARG	-	expression tag	UNP Q9UYX8
E	-9	GLY	-	expression tag	UNP Q9UYX8
E	-8	SER	-	expression tag	UNP Q9UYX8
E	-7	HIS	-	expression tag	UNP Q9UYX8
E	-6	HIS	-	expression tag	UNP Q9UYX8
E	-5	HIS	-	expression tag	UNP Q9UYX8
E	-4	HIS	-	expression tag	UNP Q9UYX8
E	-3	HIS	-	expression tag	UNP Q9UYX8
E	-2	HIS	-	expression tag	UNP Q9UYX8
E	-1	GLY	-	expression tag	UNP Q9UYX8
E	0	SER	-	expression tag	UNP Q9UYX8

- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*CP*GP*GP*GP*CP*CP*GP*AP*GP*CP*CP*GP*TP*GP*CP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	P	18	369	172	71	108	18	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(P*AP*GP*CP*AP*CP*GP*GP*CP*TP*CP*GP*GP*CP*CP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	T	16	328	153	63	96	16	0	0

- Molecule 5 is a protein called DP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	1191	9535	6102	1636	1756	41	1	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

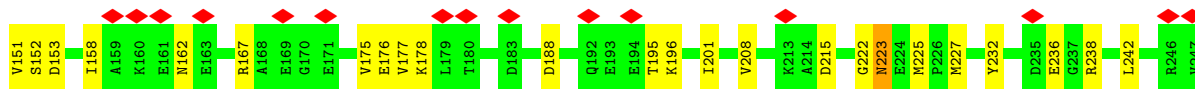
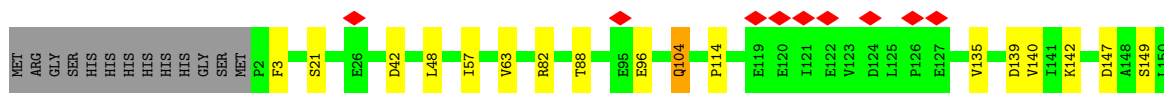
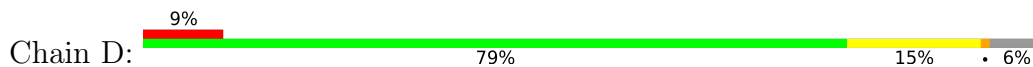
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	2	2	2	0
6	B	1	1	1	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

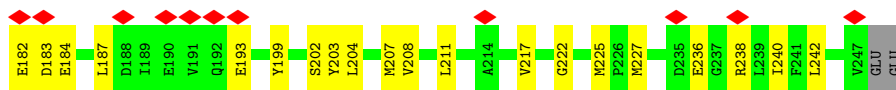
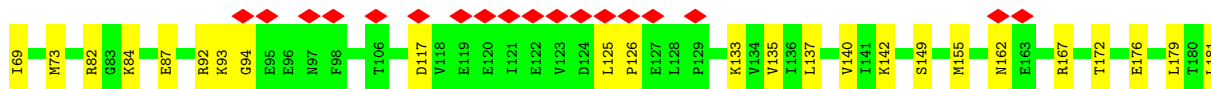
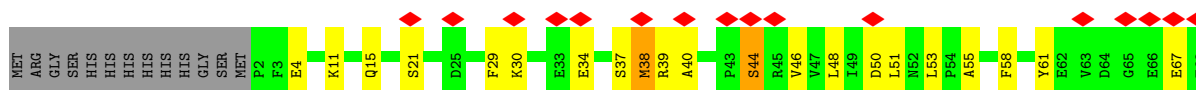
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
7	B	3	3	3	0



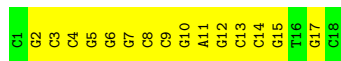
• Molecule 2: DNA polymerase sliding clamp



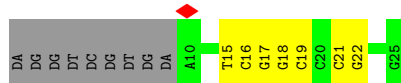
• Molecule 2: DNA polymerase sliding clamp



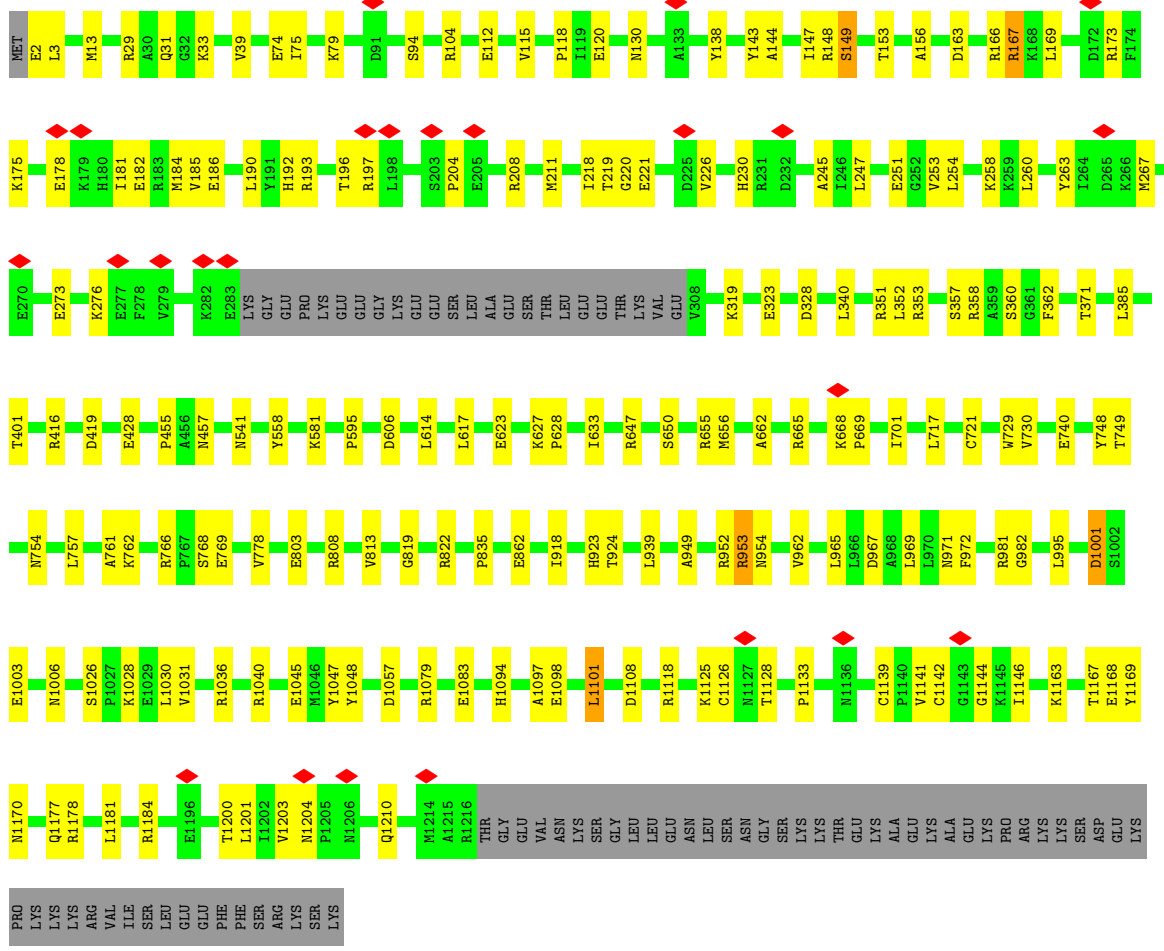
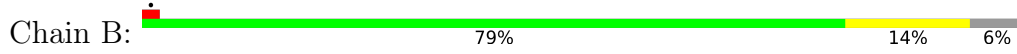
• Molecule 3: DNA (5'-D(P*CP*CP*GP*GP*GP*CP*CP*GP*AP*GP*CP*CP*GP*TP*GP*C P*TP*TP*T)-3')



• Molecule 4: DNA (5'-D(P*AP*GP*CP*AP*CP*GP*GP*CP*TP*CP*GP*GP*CP*CP*CP*G P*G)-3')



• Molecule 5: DP2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	496901	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.999	Depositor
Minimum map value	-1.263	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	344.0, 344.0, 344.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/3653	0.48	0/4960
2	C	0.26	0/1964	0.51	0/2642
2	D	0.25	0/1964	0.50	0/2642
2	E	0.25	0/1964	0.50	0/2642
3	P	0.57	0/413	0.80	0/635
4	T	0.57	0/367	0.79	0/564
5	B	0.26	0/9740	0.50	0/13161
All	All	0.28	0/20065	0.51	0/27246

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3565	0	3620	46	0
2	C	1939	0	1977	28	0
2	D	1939	0	1977	18	0
2	E	1939	0	1977	38	0
3	P	369	0	200	16	0
4	T	328	0	178	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	9535	0	9652	94	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
7	B	3	0	0	0	0
All	All	19620	0	19581	232	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:10:DG:H2''	3:P:11:DA:H5''	1.68	0.75
2:C:135:VAL:HG22	2:C:218:THR:HG22	1.74	0.70
2:E:162:ASN:HD22	2:E:181:LEU:HD11	1.55	0.70
5:B:1139:CYS:HB3	5:B:1142:CYS:HB2	1.74	0.68
2:D:57:ILE:HD11	2:D:236:GLU:HB2	1.76	0.68
5:B:1097:ALA:O	5:B:1101:LEU:HB2	1.94	0.67
5:B:181:ILE:O	5:B:185:VAL:HG23	1.95	0.66
1:A:369:CYS:HB2	1:A:619:CYS:HB2	1.79	0.65
1:A:182:ILE:HD13	1:A:378:GLU:HG2	1.78	0.64
1:A:266:GLU:HG3	1:A:320:LYS:HZ2	1.62	0.64
1:A:466:GLU:OE2	5:B:1184:ARG:NH1	2.31	0.63
2:E:135:VAL:HG22	2:E:187:LEU:HD23	1.81	0.63
1:A:213:VAL:HG11	1:A:218:GLY:HA3	1.80	0.62
1:A:303:GLU:OE2	1:A:333:LYS:NZ	2.32	0.62
2:C:167:ARG:NH2	2:C:169:GLU:OE2	2.22	0.61
2:E:48:LEU:HB3	2:E:242:LEU:HB3	1.83	0.61
4:T:16:DC:H2'	4:T:17:DG:C8	2.35	0.60
2:C:139:ASP:O	2:C:143:GLU:HG2	2.02	0.60
2:E:211:LEU:HD21	2:E:217:VAL:HG21	1.84	0.59
5:B:808:ARG:HG2	5:B:813:VAL:HG23	1.84	0.59
5:B:167:ARG:NH1	5:B:167:ARG:HB2	2.17	0.58
5:B:352:LEU:O	5:B:457:ASN:ND2	2.36	0.58
1:A:595:THR:O	1:A:595:THR:OG1	2.20	0.58
5:B:729:TRP:NE1	5:B:740:GLU:OE1	2.34	0.58
5:B:1079:ARG:O	5:B:1083:GLU:HG3	2.03	0.57
2:E:11:LYS:O	2:E:15:GLN:HG3	2.05	0.57
5:B:340:LEU:HD12	5:B:655:ARG:HB2	1.86	0.57
5:B:186:GLU:OE1	5:B:230:HIS:ND1	2.26	0.57
5:B:263:TYR:O	5:B:267:MET:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLY:HA3	1:A:331:ALA:HA	1.87	0.56
3:P:7:DG:H2''	3:P:8:DC:H5''	1.87	0.56
1:A:508:VAL:HB	1:A:511:LEU:HD12	1.87	0.56
2:C:162:ASN:O	2:C:162:ASN:ND2	2.38	0.56
2:E:67:GLU:OE1	2:E:67:GLU:N	2.39	0.56
1:A:564:TYR:HE1	1:A:600:PRO:HG3	1.72	0.55
5:B:730:VAL:HG11	5:B:761:ALA:HB2	1.87	0.55
1:A:191:VAL:HG11	1:A:395:ARG:HE	1.72	0.55
2:E:140:VAL:HG11	2:E:179:LEU:HD11	1.87	0.55
5:B:1126:CYS:HB2	5:B:1128:THR:HG22	1.87	0.55
2:C:23:LEU:HD22	2:C:47:VAL:HG11	1.89	0.54
2:E:93:LYS:NZ	2:E:94:GLY:O	2.39	0.54
2:D:158:ILE:HG23	2:D:196:LYS:HG3	1.90	0.54
5:B:149:SER:O	5:B:149:SER:OG	2.18	0.54
1:A:264:ASP:OD1	1:A:264:ASP:N	2.40	0.54
1:A:584:THR:OG1	1:A:585:GLU:N	2.40	0.53
5:B:148:ARG:HG2	5:B:247:LEU:HD23	1.89	0.53
2:C:69:ILE:HB	2:C:115:LEU:HD11	1.90	0.53
2:E:39:ARG:HB2	2:E:39:ARG:HH11	1.72	0.53
1:A:369:CYS:HB3	1:A:619:CYS:SG	2.49	0.53
1:A:590:VAL:HG23	1:A:592:ILE:HG13	1.91	0.53
5:B:204:PRO:O	5:B:208:ARG:HG3	2.08	0.53
5:B:178:GLU:O	5:B:182:GLU:HG2	2.09	0.52
1:A:385:GLU:N	1:A:385:GLU:OE1	2.42	0.52
2:C:217:VAL:HG12	2:C:231:TYR:HB3	1.91	0.52
2:E:30:LYS:HG2	2:E:37:SER:HB3	1.92	0.52
5:B:143:TYR:HE2	5:B:218:ILE:HG23	1.74	0.52
5:B:803:GLU:N	5:B:803:GLU:OE1	2.41	0.52
5:B:662:ALA:HB3	5:B:939:LEU:HD22	1.90	0.52
5:B:273:GLU:HA	5:B:276[B]:LYS:HE3	1.92	0.52
1:A:476:ASN:OD1	1:A:476:ASN:N	2.38	0.52
2:C:64:ASP:OD1	2:C:64:ASP:N	2.37	0.52
2:D:152:SER:OG	2:D:153:ASP:N	2.42	0.52
2:C:84:LYS:HB2	2:C:87:GLU:HG3	1.90	0.52
2:C:147:ASP:OD1	2:E:82:ARG:NE	2.42	0.52
5:B:1094:HIS:ND1	5:B:1170:ASN:OD1	2.41	0.52
5:B:184:MET:HG3	5:B:211:MET:SD	2.50	0.51
2:D:167:ARG:HG2	2:D:176:GLU:HG3	1.91	0.51
1:A:193:ILE:HB	1:A:397:LYS:HD2	1.93	0.51
2:E:39:ARG:HB2	2:E:39:ARG:NH1	2.25	0.51
5:B:457:ASN:HB3	5:B:647:ARG:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:113:LEU:HD12	2:C:114:PRO:HD2	1.93	0.50
3:P:5:DG:H4'	3:P:6:DG:OP1	2.10	0.50
5:B:104:ARG:NH1	5:B:118:PRO:O	2.44	0.50
2:D:139:ASP:OD1	2:D:140:VAL:N	2.45	0.50
5:B:416:ARG:HG3	5:B:595:PRO:HG3	1.93	0.50
2:E:29:PHE:O	2:E:69:ILE:N	2.40	0.50
1:A:318:ALA:HB3	1:A:335:TYR:HB2	1.94	0.49
5:B:75:ILE:O	5:B:79:LYS:HG2	2.12	0.49
2:C:242:LEU:HD23	5:B:1201:LEU:HD21	1.94	0.49
5:B:541:ASN:OD1	5:B:633:ILE:HG13	2.11	0.49
2:C:218:THR:OG1	2:C:230:GLU:HB2	2.12	0.49
2:E:203:TYR:O	2:E:207:MET:HG3	2.12	0.49
4:T:18:DG:H2''	4:T:19:DC:O5'	2.13	0.49
2:C:53:LEU:HB3	2:C:58:PHE:HE1	1.76	0.49
1:A:231:LEU:HB2	1:A:542:ASP:O	2.13	0.49
1:A:265:GLU:OE1	1:A:265:GLU:N	2.46	0.48
2:C:6:VAL:HG22	2:C:90:ILE:HG12	1.96	0.48
5:B:218:ILE:HG22	5:B:245:ALA:HB1	1.96	0.48
2:C:31:VAL:HA	2:C:36:ILE:HA	1.96	0.48
5:B:163:ASP:O	5:B:166:ARG:HG3	2.14	0.48
5:B:954:ASN:ND2	5:B:1003:GLU:OE2	2.47	0.48
2:D:88:THR:HB	2:D:104:GLN:HB3	1.95	0.48
5:B:112:GLU:HG3	5:B:952:ARG:HH22	1.78	0.48
5:B:31:GLN:OE1	5:B:33:LYS:NZ	2.46	0.48
1:A:350:GLU:H	1:A:350:GLU:CD	2.17	0.47
2:D:114:PRO:HG2	2:E:172:THR:HB	1.95	0.47
2:E:167:ARG:HB3	2:E:167:ARG:NH1	2.30	0.47
2:D:151:VAL:HG21	2:D:175:VAL:HG23	1.95	0.47
2:D:3:PHE:HB2	2:D:63:VAL:HG22	1.95	0.47
2:E:222:GLY:HA3	2:E:225:MET:HE2	1.97	0.47
1:A:587:GLN:OE1	1:A:594:PRO:HG3	2.15	0.47
5:B:115:VAL:HG23	5:B:923:HIS:O	2.15	0.47
2:C:238:ARG:HH11	2:C:240:ILE:HD11	1.80	0.47
3:P:12:DG:H2'	3:P:13:DC:C6	2.50	0.46
5:B:455:PRO:O	5:B:650:SER:OG	2.28	0.46
5:B:1125:LYS:HB3	5:B:1125:LYS:HE3	1.78	0.46
1:A:487:ARG:NH2	1:A:492:ASP:OD2	2.48	0.46
2:E:117:ASP:OD1	2:E:117:ASP:N	2.45	0.46
3:P:9:DC:H2'	3:P:10:DG:C8	2.50	0.46
2:E:44:SER:HB3	2:E:46:VAL:HG12	1.98	0.46
2:E:38:MET:HB3	2:E:51:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:84:LYS:H	2:E:87:GLU:HG3	1.81	0.46
3:P:6:DG:H2''	3:P:7:DG:C8	2.51	0.46
5:B:143:TYR:CE2	5:B:218:ILE:HG23	2.51	0.46
2:D:48:LEU:HB3	2:D:242:LEU:HB3	1.98	0.45
2:E:142:LYS:HG3	2:E:208:VAL:HG12	1.98	0.45
5:B:219:THR:OG1	5:B:220:GLY:N	2.49	0.45
2:E:34:GLU:O	2:E:55:ALA:N	2.47	0.45
5:B:1040:ARG:HD3	5:B:1045:GLU:O	2.16	0.45
2:E:204:LEU:O	2:E:208:VAL:HG23	2.16	0.45
5:B:1142:CYS:HB3	5:B:1144:GLY:H	1.82	0.45
5:B:819:GLY:O	5:B:971:ASN:HB3	2.17	0.45
2:E:38:MET:SD	2:E:39:ARG:N	2.90	0.45
4:T:21:DC:H2''	4:T:22:DG:H5''	1.98	0.45
5:B:1141:VAL:HG22	5:B:1141:VAL:O	2.17	0.45
1:A:392:ILE:O	1:A:396:VAL:HG23	2.16	0.45
1:A:439:PRO:HD2	1:A:442:ILE:HD12	1.97	0.45
2:E:39:ARG:NH2	2:E:50:ASP:OD1	2.49	0.45
2:E:238:ARG:HD2	2:E:240:ILE:HD11	1.98	0.45
4:T:15:DT:H2'	4:T:16:DC:C6	2.52	0.45
5:B:627:LYS:HG2	5:B:628:PRO:HD2	1.98	0.45
5:B:1203:VAL:HG22	5:B:1204:ASN:H	1.82	0.45
3:P:17:DG:H22	5:B:193:ARG:NH2	2.15	0.45
5:B:668:LYS:HB3	5:B:669:PRO:HD3	1.99	0.45
1:A:369:CYS:CB	1:A:619:CYS:SG	3.05	0.44
2:C:34:GLU:OE2	2:C:34:GLU:HA	2.17	0.44
5:B:221:GLU:OE1	5:B:221:GLU:N	2.40	0.44
5:B:120:GLU:OE2	5:B:982:GLY:N	2.27	0.44
3:P:2:DG:H2''	3:P:3:DC:O5'	2.17	0.44
5:B:192:HIS:CD2	5:B:197:ARG:HA	2.53	0.44
1:A:423:ASP:OD1	5:B:1177:GLN:NE2	2.34	0.44
5:B:953:ARG:HD2	5:B:953:ARG:HA	1.74	0.44
2:D:222:GLY:HA3	2:D:225:MET:CE	2.48	0.44
2:C:35:GLY:HA2	2:C:61:TYR:HE2	1.83	0.44
4:T:18:DG:H4'	4:T:19:DC:OP1	2.16	0.44
5:B:130:ASN:HD21	5:B:175:LYS:H	1.66	0.44
1:A:359:SER:OG	1:A:360:ASP:OD1	2.36	0.44
1:A:502:GLU:OE2	1:A:560:HIS:NE2	2.50	0.44
2:E:137:LEU:HD12	2:E:187:LEU:HD21	2.00	0.44
3:P:13:DC:H2'	3:P:14:DC:C6	2.53	0.44
5:B:558:TYR:CD2	5:B:581:LYS:HD2	2.53	0.43
2:D:195:THR:HA	2:D:223:ASN:ND2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6:DG:H5''	3:P:6:DG:H8	1.83	0.43
1:A:306:ARG:NE	1:A:306:ARG:O	2.51	0.43
1:A:355:ALA:HB3	1:A:602:VAL:HG22	2.00	0.43
1:A:534:GLY:HA2	5:B:1118:ARG:HB2	1.99	0.43
2:E:199:TYR:CZ	2:E:227:MET:HB3	2.53	0.43
5:B:717:LEU:HD23	5:B:717:LEU:HA	1.87	0.43
5:B:1146:ILE:HD13	5:B:1146:ILE:HA	1.86	0.43
2:E:4:GLU:HG3	2:E:92:ARG:HH11	1.84	0.43
3:P:15:DG:N2	5:B:1178:ARG:HH12	2.16	0.43
5:B:319:LYS:O	5:B:323:GLU:HG2	2.19	0.43
5:B:144:ALA:O	5:B:147:ILE:HG22	2.19	0.43
1:A:215:ASN:OD1	1:A:217:SER:N	2.46	0.42
1:A:288:GLU:HB2	1:A:293:ILE:HG23	2.01	0.42
2:E:187:LEU:H	2:E:187:LEU:HD22	1.84	0.42
5:B:1167:THR:HG23	5:B:1168:GLU:HG2	2.01	0.42
5:B:1210:GLN:H	5:B:1210:GLN:HG2	1.62	0.42
5:B:169:LEU:HD23	5:B:169:LEU:HA	1.90	0.42
5:B:1028:LYS:HA	5:B:1031:VAL:HG23	2.01	0.42
1:A:358:ILE:HD11	1:A:376:PHE:CE2	2.55	0.42
3:P:5:DG:H2''	3:P:6:DG:H5''	2.00	0.42
5:B:351:ARG:NH1	5:B:647:ARG:O	2.53	0.42
2:C:82:ARG:HD3	2:D:147:ASP:OD1	2.19	0.42
5:B:614:LEU:HD23	5:B:614:LEU:HA	1.89	0.42
5:B:748:TYR:HA	5:B:757:LEU:HD12	2.02	0.42
2:E:37:SER:OG	2:E:38:MET:N	2.53	0.42
1:A:265:GLU:HG2	1:A:267:VAL:HG13	2.00	0.42
1:A:528:HIS:HD2	1:A:548:VAL:HG22	1.85	0.42
2:C:193:GLU:HG3	2:C:194:GLU:N	2.35	0.42
5:B:247:LEU:HD12	5:B:247:LEU:HA	1.67	0.42
5:B:258:LYS:HE2	5:B:258:LYS:HB3	1.82	0.42
3:P:15:DG:H21	5:B:1178:ARG:HH12	1.67	0.42
5:B:156:ALA:HB1	5:B:260:LEU:HD22	2.01	0.42
5:B:1098:GLU:HG2	5:B:1169:TYR:HB2	2.02	0.42
2:C:159:ALA:HB3	2:C:195:THR:HB	2.02	0.42
5:B:357:SER:OG	5:B:358:ARG:N	2.52	0.42
2:C:146:LYS:HE2	2:E:82:ARG:NH1	2.34	0.41
2:E:58:PHE:HB2	2:E:61:TYR:HB2	2.01	0.41
5:B:949:ALA:HB1	5:B:1001:ASP:HB2	2.03	0.41
1:A:452:ASP:N	1:A:452:ASP:OD1	2.53	0.41
2:C:228:GLN:HA	2:C:241:PHE:O	2.20	0.41
2:D:149:SER:HB2	2:D:201:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:109:ARG:HG2	2:D:177:VAL:HG13	2.03	0.41
1:A:228:TYR:HB3	5:B:1133:PRO:HG3	2.02	0.41
5:B:115:VAL:HA	5:B:924:THR:HA	2.02	0.41
5:B:918:ILE:HD11	5:B:965:LEU:HD12	2.03	0.41
1:A:176:LYS:HB2	1:A:430:ALA:HB2	2.03	0.41
2:E:38:MET:HE1	2:E:40:ALA:HB2	2.02	0.41
3:P:3:DC:H2''	3:P:4:DC:C6	2.55	0.41
5:B:2:GLU:HB3	5:B:3:LEU:H	1.73	0.41
5:B:74:GLU:OE1	5:B:74:GLU:N	2.51	0.41
5:B:1163:LYS:O	5:B:1167:THR:HG22	2.20	0.41
1:A:312:LEU:HD12	1:A:532:THR:OG1	2.20	0.41
2:E:183:ASP:OD1	2:E:184:GLU:N	2.54	0.41
5:B:253:VAL:HG23	5:B:254:LEU:HD13	2.03	0.41
2:C:233:ILE:HG23	2:C:237:GLY:HA3	2.03	0.41
2:D:135:VAL:HB	2:D:188:ASP:HB2	2.03	0.41
2:D:142:LYS:HG3	2:D:208:VAL:HG12	2.03	0.41
2:E:182:GLU:OE1	2:E:182:GLU:N	2.53	0.41
3:P:9:DC:H2'	3:P:10:DG:H8	1.85	0.41
5:B:29:ARG:NH2	5:B:972:PHE:O	2.54	0.41
5:B:39:VAL:HG11	5:B:969:LEU:HD22	2.03	0.41
5:B:190:LEU:HD21	5:B:226:VAL:HG11	2.03	0.41
5:B:192:HIS:HA	5:B:196:THR:O	2.21	0.41
1:A:279:THR:HG23	1:A:282:GLY:H	1.84	0.41
2:D:222:GLY:HA3	2:D:225:MET:HE2	2.02	0.41
3:P:11:DA:H2'	3:P:12:DG:C8	2.56	0.41
5:B:835:PRO:HB2	5:B:862:GLU:HG2	2.03	0.41
5:B:665:ARG:HH21	5:B:822:ARG:HD2	1.86	0.40
5:B:954:ASN:ND2	5:B:954:ASN:O	2.55	0.40
5:B:1006:ASN:OD1	5:B:1036:ARG:NH1	2.53	0.40
2:C:204:LEU:O	2:C:208:VAL:HG22	2.21	0.40
2:E:125:LEU:HD12	2:E:126:PRO:HD2	2.03	0.40
5:B:112:GLU:HG3	5:B:952:ARG:NH2	2.36	0.40
5:B:1098:GLU:N	5:B:1098:GLU:OE1	2.54	0.40
1:A:296:VAL:HG22	1:A:329:PHE:HB3	2.02	0.40
1:A:438:VAL:HG21	1:A:444:MET:SD	2.62	0.40
2:C:42:ASP:OD1	2:C:44:SER:HB2	2.22	0.40
1:A:306:ARG:NH2	1:A:309:PHE:HB3	2.35	0.40
5:B:328:ASP:O	5:B:328:ASP:OD1	2.39	0.40
5:B:995:LEU:HD12	5:B:995:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/662 (67%)	424 (95%)	21 (5%)	0	100	100
2	C	244/261 (94%)	237 (97%)	7 (3%)	0	100	100
2	D	244/261 (94%)	238 (98%)	6 (2%)	0	100	100
2	E	244/261 (94%)	237 (97%)	7 (3%)	0	100	100
5	B	1188/1270 (94%)	1138 (96%)	50 (4%)	0	100	100
All	All	2365/2715 (87%)	2274 (96%)	91 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	392/573 (68%)	375 (96%)	17 (4%)	29	62
2	C	214/227 (94%)	193 (90%)	21 (10%)	8	24
2	D	214/227 (94%)	202 (94%)	12 (6%)	21	52
2	E	214/227 (94%)	202 (94%)	12 (6%)	21	52
5	B	1024/1094 (94%)	981 (96%)	43 (4%)	30	63
All	All	2058/2348 (88%)	1953 (95%)	105 (5%)	27	56

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	GLU
1	A	202	ASP
1	A	207	LYS
1	A	209	ARG
1	A	237	SER
1	A	289	ASP
1	A	298	LEU
1	A	306	ARG
1	A	312	LEU
1	A	371	LYS
1	A	450	ASN
1	A	452	ASP
1	A	475	LYS
1	A	595	THR
1	A	602	VAL
1	A	608	ARG
1	A	619	CYS
2	C	15	GLN
2	C	42	ASP
2	C	51	LEU
2	C	61	TYR
2	C	64	ASP
2	C	77	LYS
2	C	82	ARG
2	C	102	SER
2	C	115	LEU
2	C	117	ASP
2	C	154	SER
2	C	161	GLU
2	C	162	ASN
2	C	165	THR
2	C	183	ASP
2	C	187	LEU
2	C	194	GLU
2	C	201	ILE
2	C	206	ASP
2	C	223	ASN
2	C	233	ILE
2	D	21	SER
2	D	42	ASP
2	D	82	ARG
2	D	96	GLU
2	D	104	GLN

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Mol	Chain	Res	Type
2	D	162	ASN
2	D	178	LYS
2	D	215	ASP
2	D	223	ASN
2	D	227	MET
2	D	232	TYR
2	D	238	ARG
2	E	21	SER
2	E	38	MET
2	E	44	SER
2	E	53	LEU
2	E	73	MET
2	E	133	LYS
2	E	149	SER
2	E	155	MET
2	E	176	GLU
2	E	193	GLU
2	E	202	SER
2	E	236	GLU
5	B	13	MET
5	B	94	SER
5	B	138	TYR
5	B	149	SER
5	B	153	THR
5	B	167	ARG
5	B	173	ARG
5	B	251	GLU
5	B	353	ARG
5	B	360	SER
5	B	362	PHE
5	B	371	THR
5	B	385	LEU
5	B	401	THR
5	B	419	ASP
5	B	428	GLU
5	B	606	ASP
5	B	617	LEU
5	B	623	GLU
5	B	656	MET
5	B	701	ILE
5	B	721	CYS
5	B	749	THR

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Mol	Chain	Res	Type
5	B	754	ASN
5	B	762	LYS
5	B	766	ARG
5	B	768	SER
5	B	769	GLU
5	B	778	VAL
5	B	953	ARG
5	B	962	VAL
5	B	967	ASP
5	B	981	ARG
5	B	1001	ASP
5	B	1026	SER
5	B	1030	LEU
5	B	1047	TYR
5	B	1048	TYR
5	B	1057	ASP
5	B	1101	LEU
5	B	1108	ASP
5	B	1181	LEU
5	B	1200	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
5	B	130	ASN
5	B	954	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

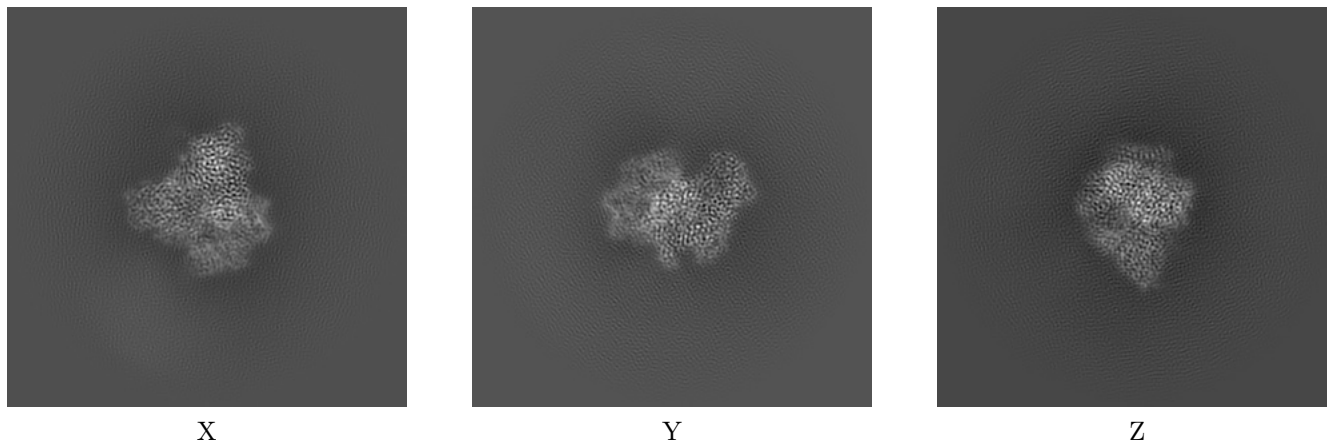
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17815. These allow visual inspection of the internal detail of the map and identification of artifacts.

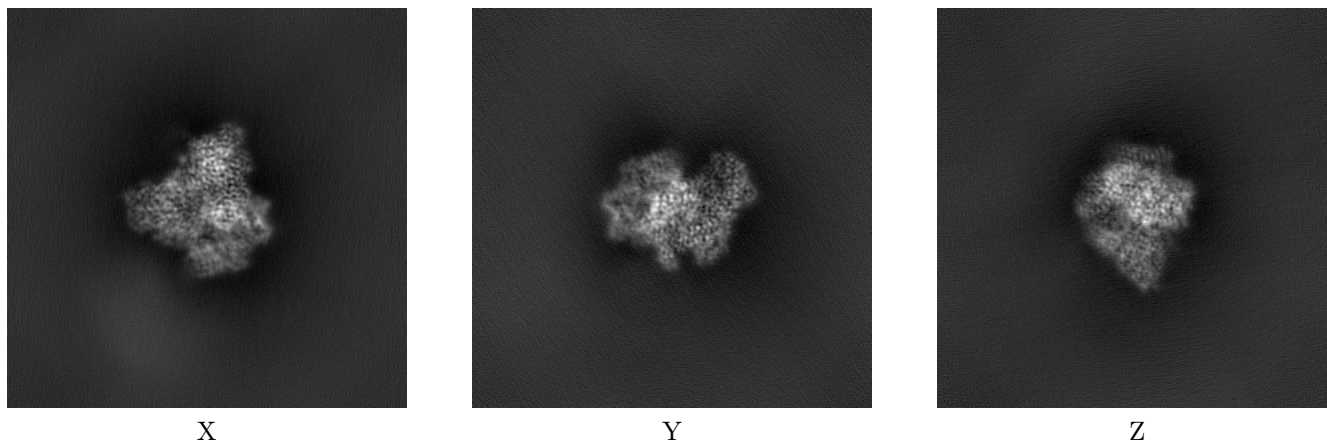
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



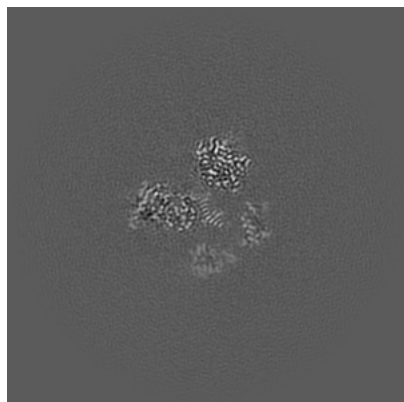
6.1.2 Raw map



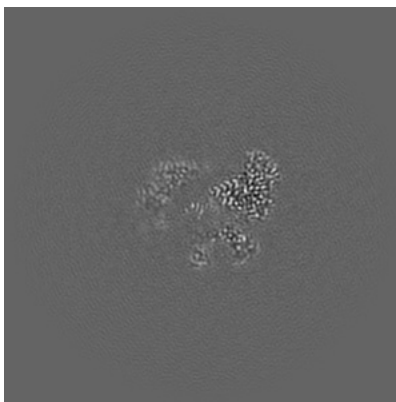
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

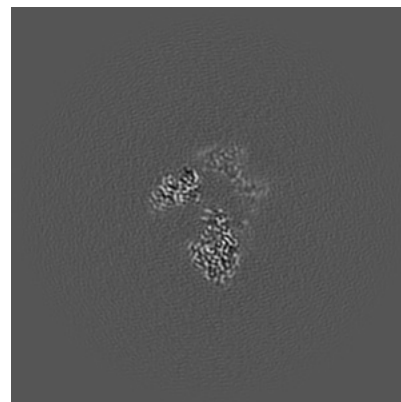
6.2.1 Primary map



X Index: 200

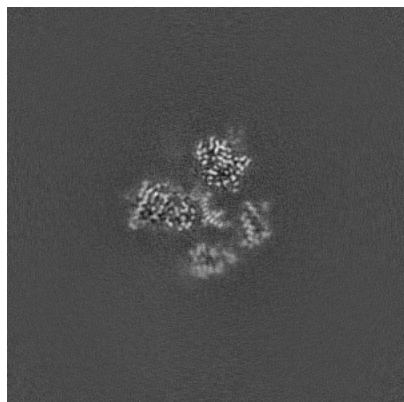


Y Index: 200

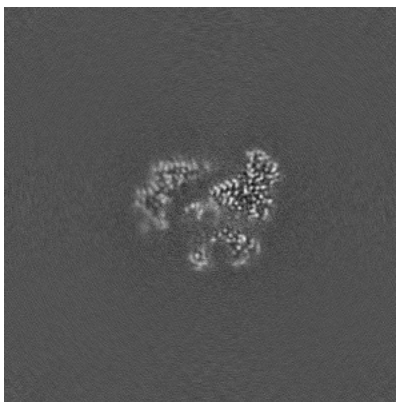


Z Index: 200

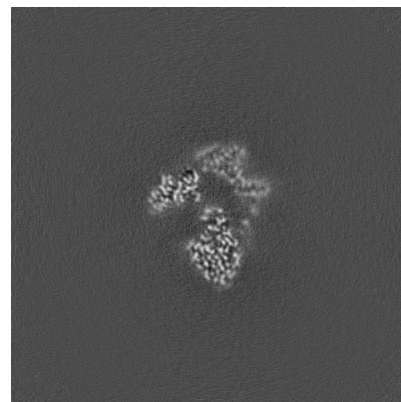
6.2.2 Raw map



X Index: 200



Y Index: 200

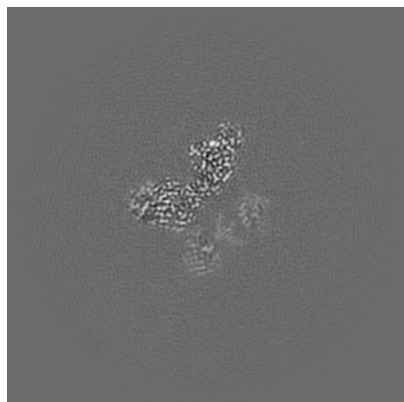


Z Index: 200

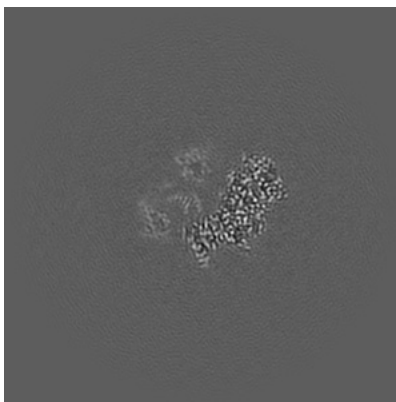
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

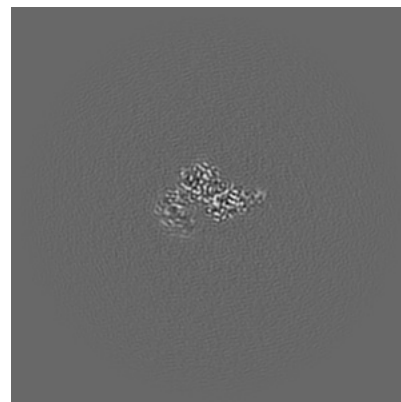
6.3.1 Primary map



X Index: 211

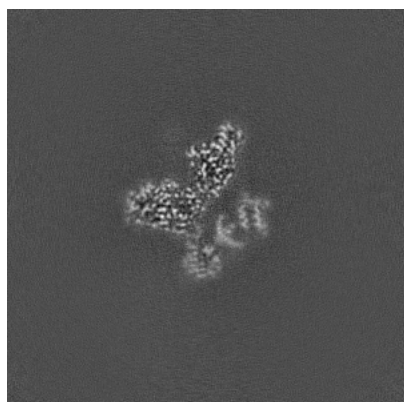


Y Index: 214

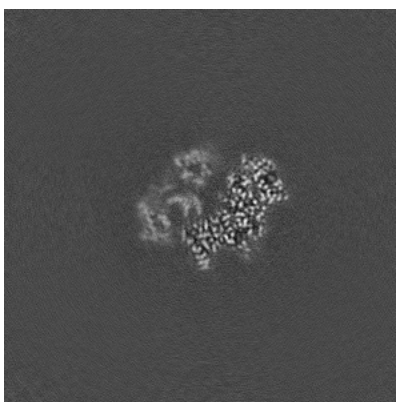


Z Index: 240

6.3.2 Raw map



X Index: 210



Y Index: 214

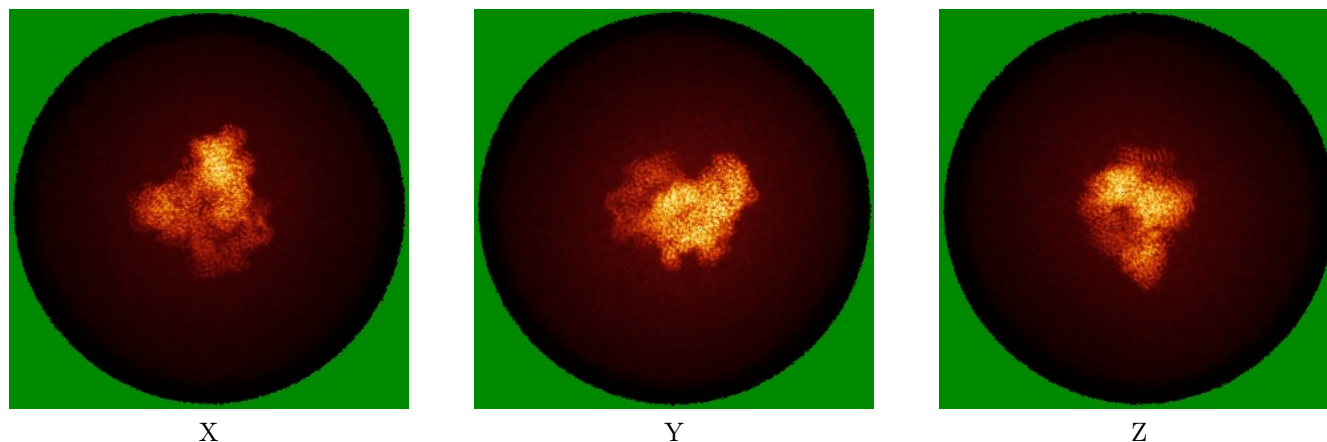


Z Index: 199

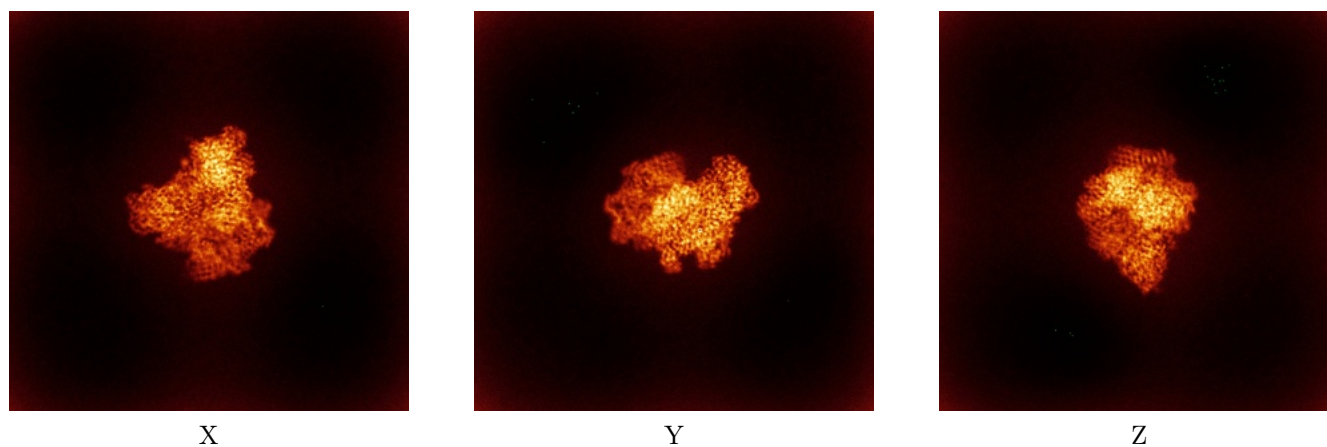
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



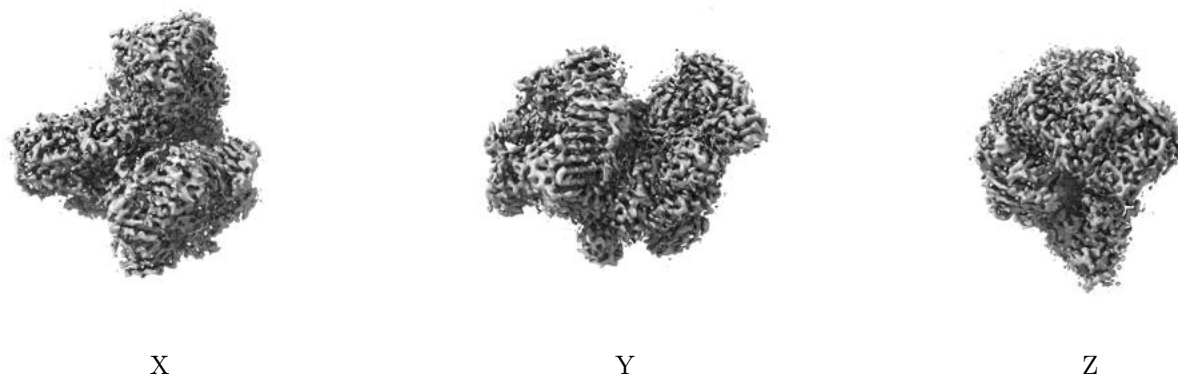
6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

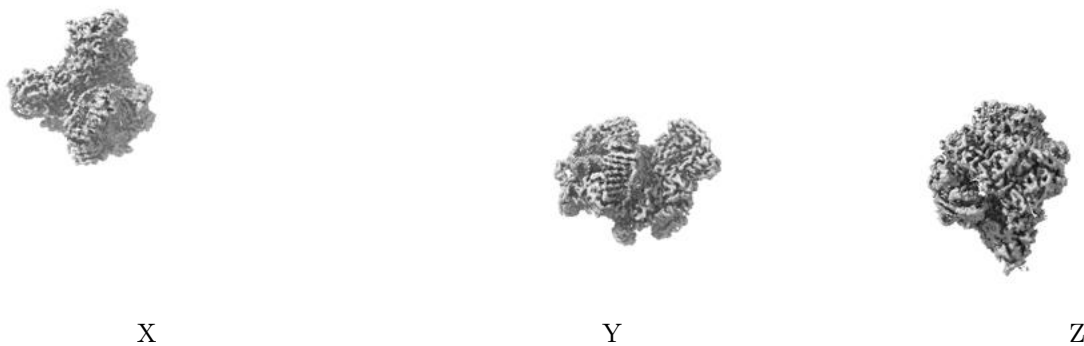
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

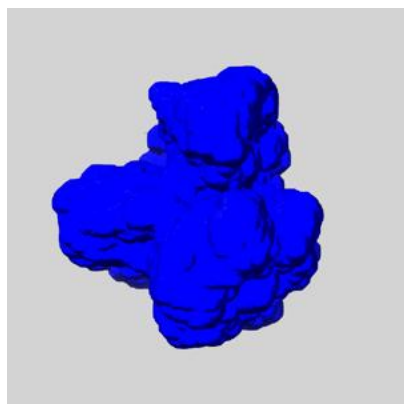
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

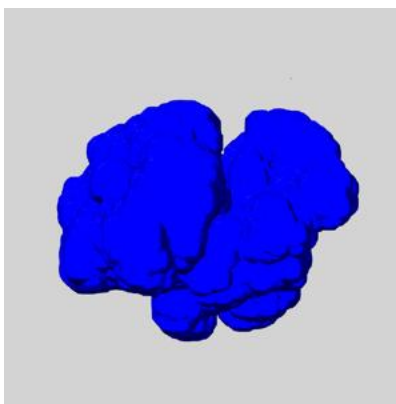
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

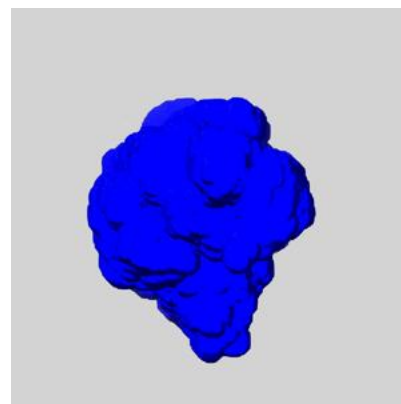
6.6.1 emd_17815_msk_1.map [i](#)



X



Y

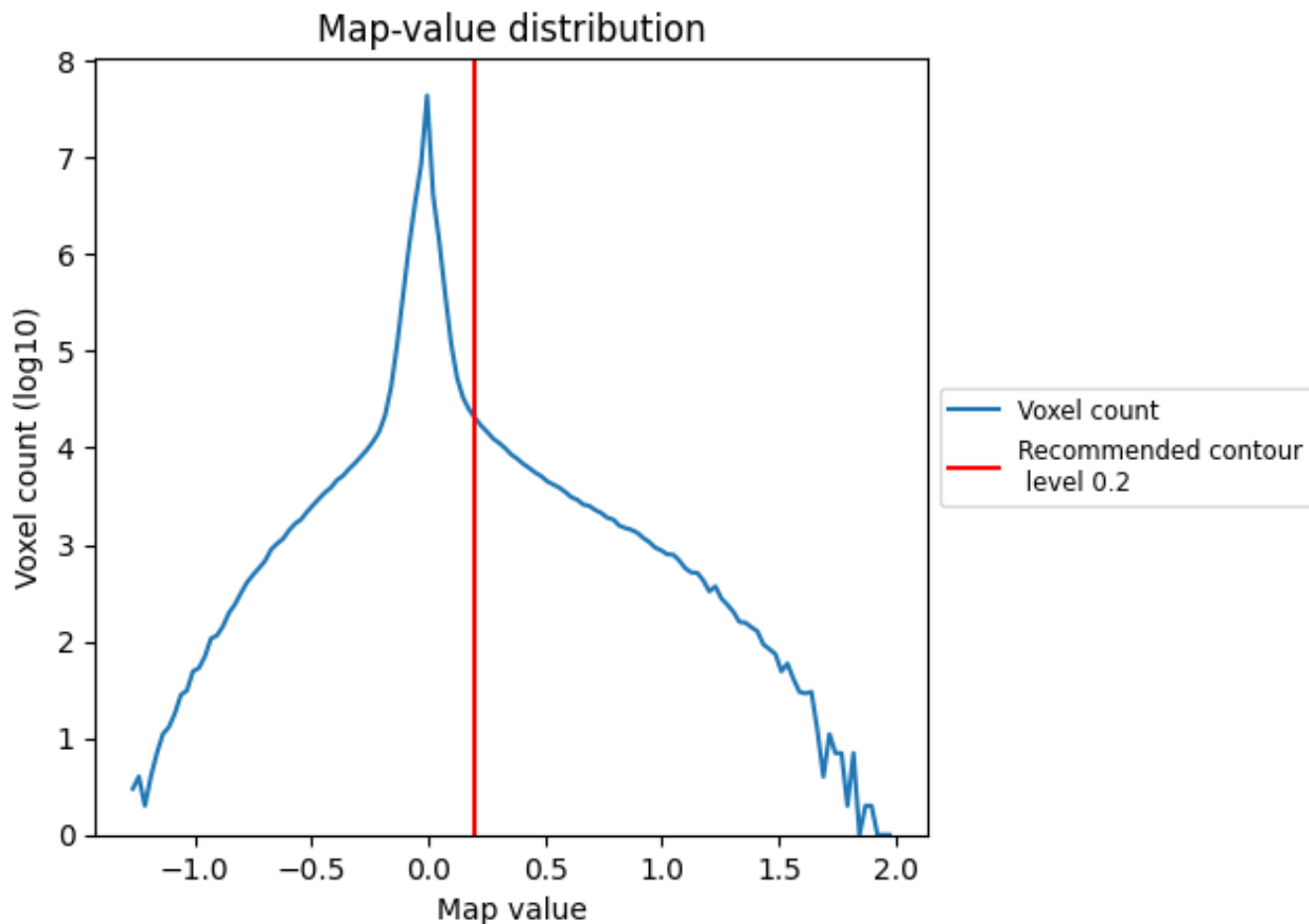


Z

7 Map analysis [i](#)

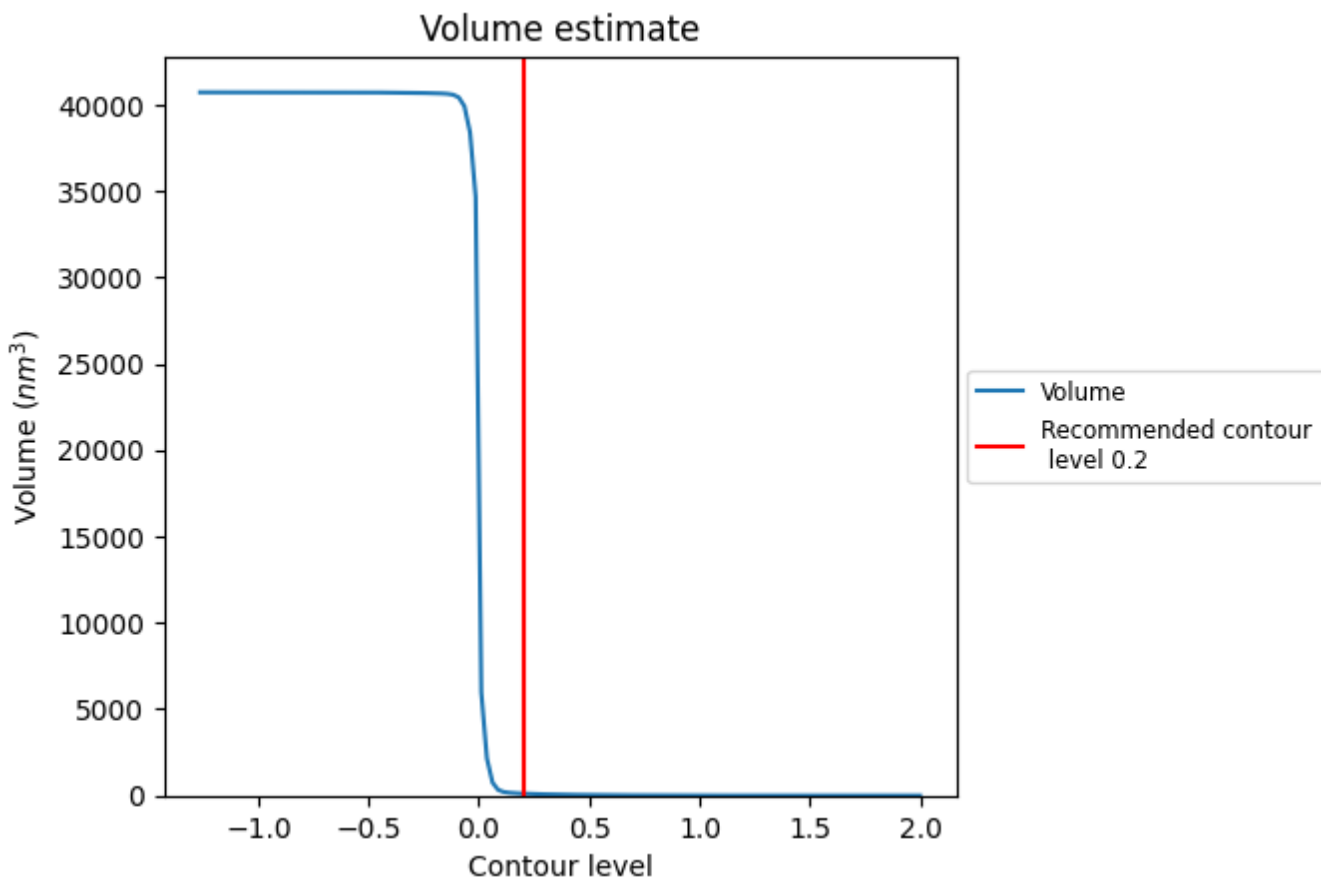
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

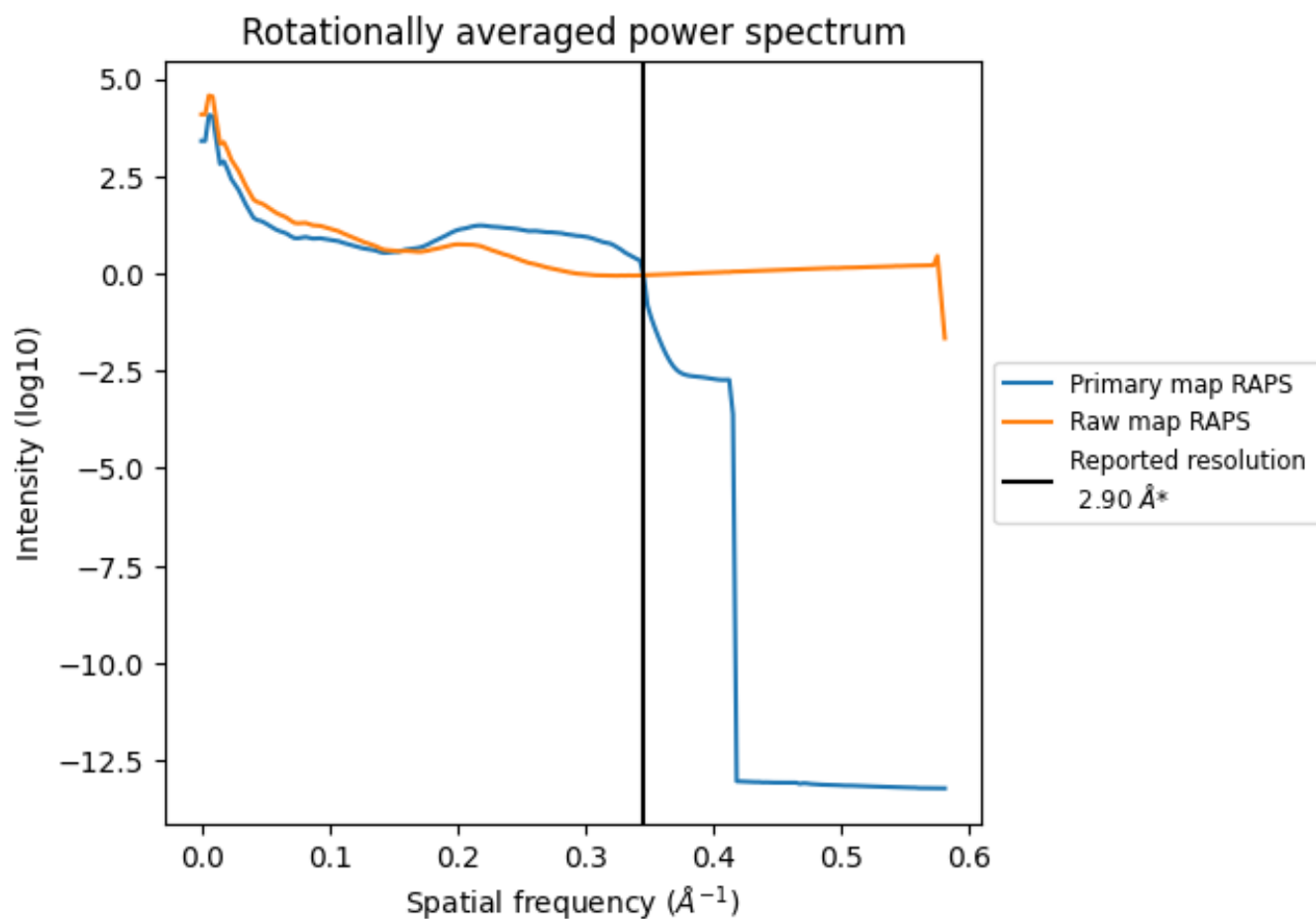
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm³; this corresponds to an approximate mass of 103 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

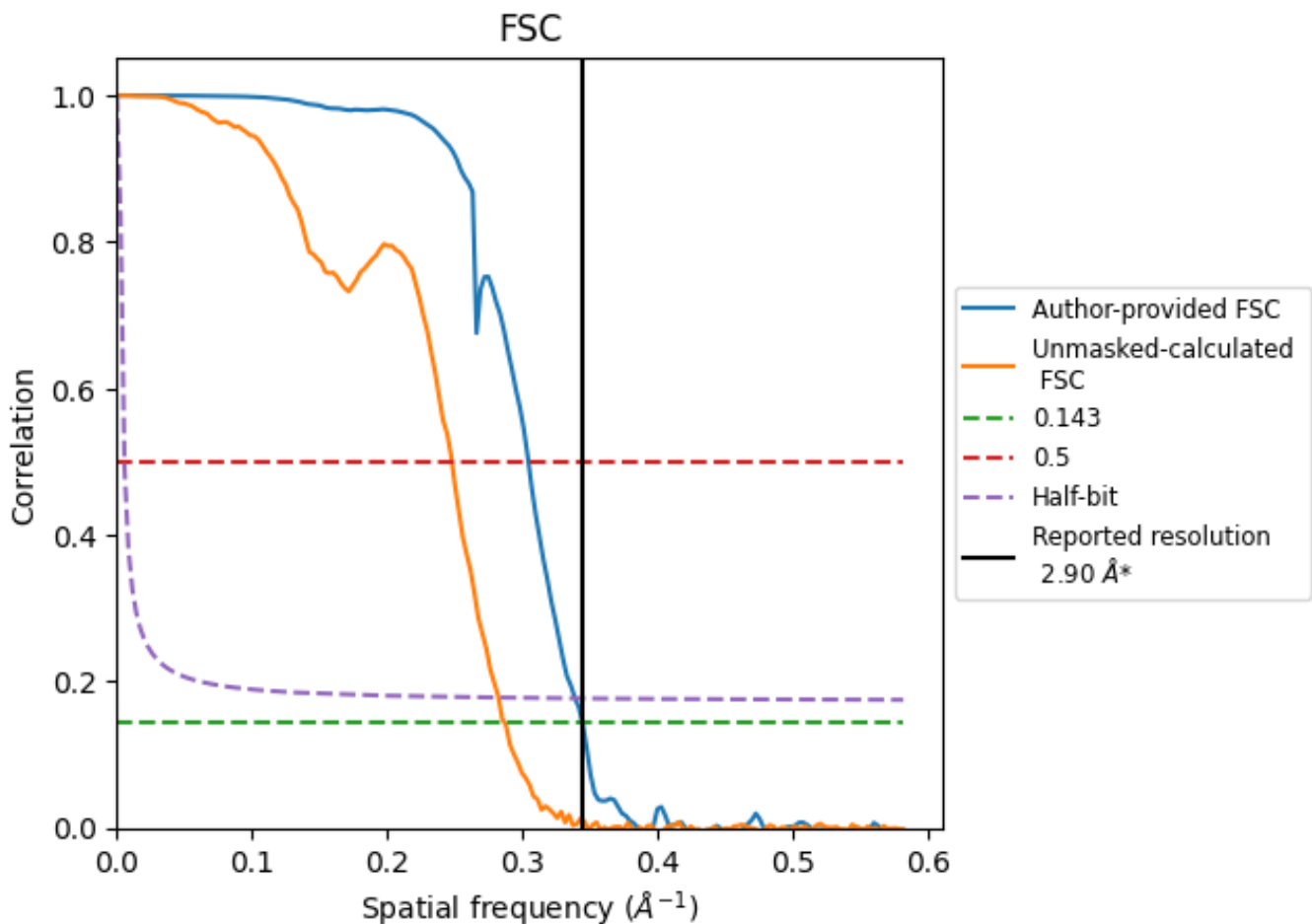


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

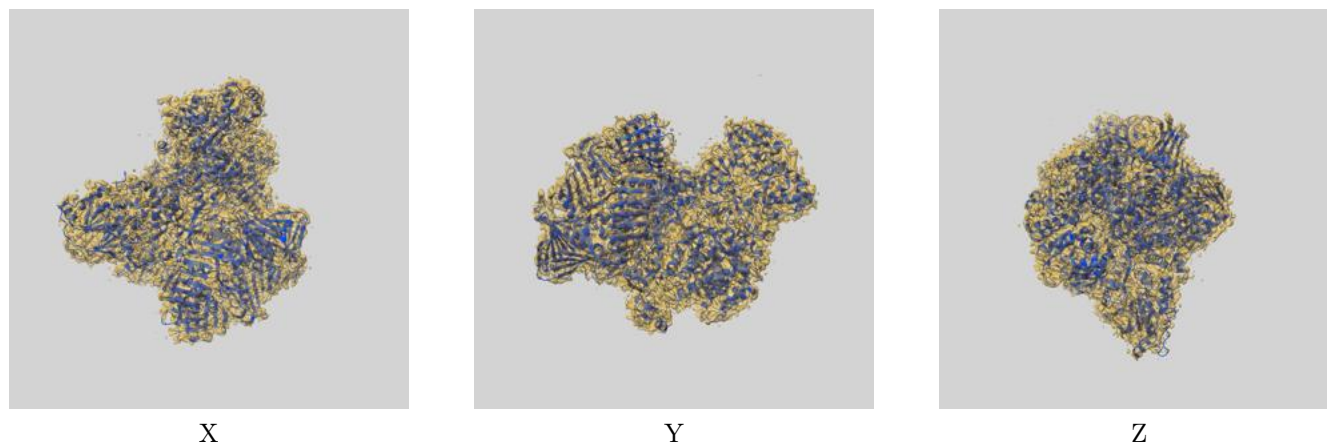
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.29	2.95
Unmasked-calculated*	3.49	4.04	3.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.49 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17815 and PDB model 8PPT. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



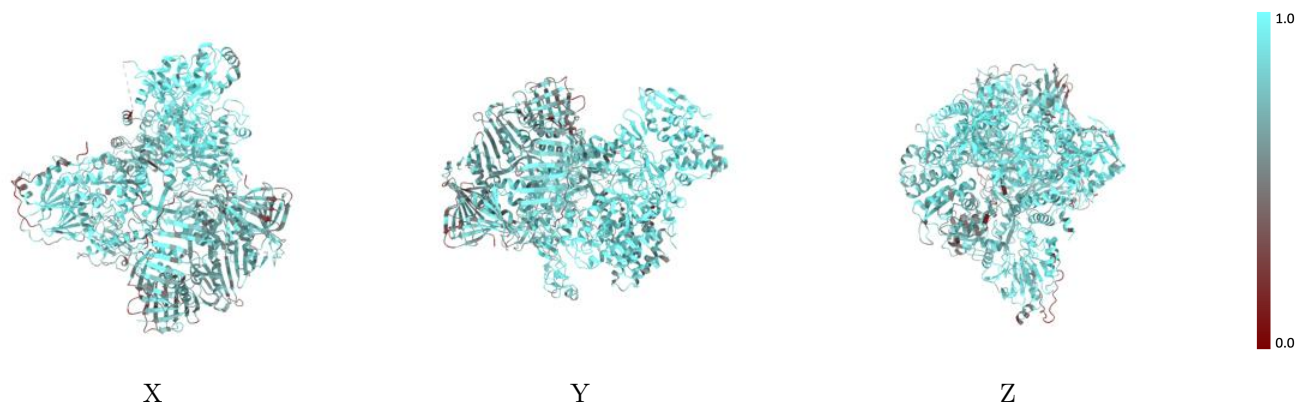
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



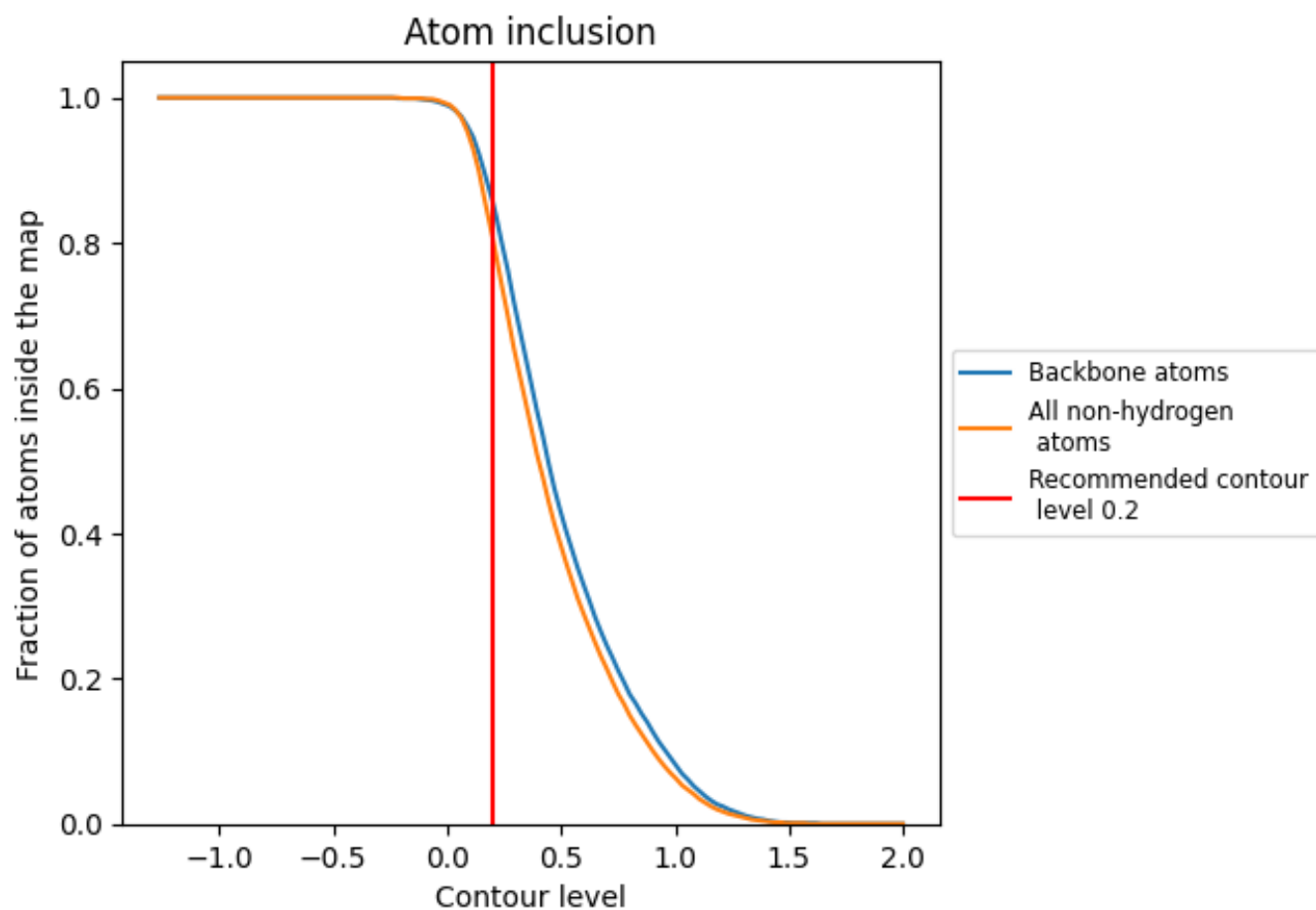
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

















9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8060	 0.5500
A	 0.8050	 0.5480
B	 0.8870	 0.5840
C	 0.6840	 0.5000
D	 0.7180	 0.5230
E	 0.6260	 0.4800
P	 0.8160	 0.5300
T	 0.7800	 0.5110

